

Physical and Interdisciplinary Regional Ocean Dynamics and Modeling Systems

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Award #: N00014-07-1-1061 - N00014-08-1-1097 (04/01/07 - 09/31/10) - **FY08**

Web: <http://mseas.mit.edu/Research/ONR6.1/index.html>, <http://mseas.mit.edu/>

LONG-TERM GOALS

This research is concerned with the fundamental understanding and modeling of complex physical, acoustical and biogeochemical oceanic dynamics and processes. New mathematical models and computational methods are created, developed and utilized for i) ocean predictions and dynamical diagnostics, ii) data assimilation and data-model comparisons, and, iii) optimization and control of autonomous ocean observation systems.

OBJECTIVES

General objectives are to:

- i) Analyze and study regional physical and acoustical-physical-biogeochemical dynamics
- ii) Incubate and develop new numerical modeling systems, including next generation ocean physics, 3D acoustics and Lagrangian coherent structures predictions
- iii) Update existing and create new nonlinear and adaptive assimilation schemes and systems, including parameter estimation
- iv) Evolve concepts and determine methodologies for regional adaptive modeling and adaptive sampling with the intent to increase predictive capabilities
- v) Quantify regional predictabilities and improve probability and uncertainty modeling
- vi) Utilize several ocean models, estimate their uncertainty statistics and fuse their estimates

APPROACH

The technical approach is rooted in the comparison and optimal combination of measurements and models via nonlinear data assimilation (DA), including the development of adaptive modeling and adaptive sampling schemes based on Error Subspace Statistical Estimation. Topics specific to the present effort include: three-dimensional acoustic modeling coupled to ocean modeling; incubator for the next-generation numerical ocean modeling; interactions of mesoscales with internal tides and waves, and mixing processes; Lagrangian coherent structures and ocean features; nonlinear data assimilation and multi-model estimations.

The regional dynamics studied involves interactions of sub-mesoscale and mesoscale ocean processes in the littoral as well as effects from large-scale processes in ocean basins. Such interactions and feedbacks with scales smaller and larger than the mesoscale need be better quantified. Investigations are generic but the focus is on specific ocean regions: the Mid-Atlantic Bight (MAB) and Shelfbreak Front region, the Chinese-Taiwanese Seas and Philippine Seas; the Monterey Bay and California

Report Documentation Page			Form Approved OMB No. 0704-0188		
Public reporting burden for the collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to a penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.					
1. REPORT DATE 30 SEP 2008		2. REPORT TYPE Annual		3. DATES COVERED 00-00-2008 to 00-00-2008	
4. TITLE AND SUBTITLE Physical And Interdisciplinary Regional Ocean Dynamics And Modeling Systems			5a. CONTRACT NUMBER		
			5b. GRANT NUMBER		
			5c. PROGRAM ELEMENT NUMBER		
6. AUTHOR(S)			5d. PROJECT NUMBER		
			5e. TASK NUMBER		
			5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Massachusetts Institute of Technology, Department of Mechanical Engineering, Ocean Science and Engineering, Room 5-207B; 77 Massachusetts Avenue, Cambridge, MA, 02139-4307			8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)			10. SPONSOR/MONITOR'S ACRONYM(S)		
			11. SPONSOR/MONITOR'S REPORT NUMBER(S)		
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited					
13. SUPPLEMENTARY NOTES code 1 only					
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15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT Same as Report (SAR)	18. NUMBER OF PAGES 10	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			

Current System (CCS) region, the Massachusetts Bay/New England shelf region, and the Mediterranean and Black Seas. Several of these regions have been or are investigated under other collaborative efforts. The present proposal is leveraging these other projects, aiming to carry out the creative and fundamental research necessary for major advances and forward leaps.

The research consists of two inter-related thematic areas: Modeling System and Ocean Dynamics. The Modeling System research involves the incubation of new ocean modeling methods and schemes, the investigation of 3D acoustic modeling, continued efforts in interdisciplinary nonlinear and adaptive DA and parameter estimation, the estimation of model uncertainties and combination of multiple models and the development of self-modifying models that learn from data. The Ocean Dynamics research includes the applications of these modeling systems to generic ocean process studies and specific ocean regions. It involves studies of frontal systems and their multiscale interactions, of coastal bays and their shelf interactions, and of semi-enclosed seas and their water-mass interactions.

WORK COMPLETED

Unstructured Grid Modeling: The Discontinuous Galerkin Finite Element Method (DGFEM) was implemented in MATLAB to solve advection-diffusion-reaction equations in 2D space. Several test cases were conducted to evaluate the accuracy of DGFEM for advection-dominated flows. Specifically, the effects of time discretization, time integration schemes, space discretization, and order of basis functions were examined. Following these studies, an idealized biogeochemical test case was implemented to study the behavior of DGFEM with non-linear source terms. For this study, a simple Nutrient-Phytoplankton-Zooplankton (NPZ) model was used. After obtaining stable, convergent results, the DGFEM implementation was extended to use variable orders of basis functions on the same grid. This implementation allows different constituents to use different basis functions on the same elements. Results were presented at the unstructured modeling workshop in Halifax, Ca.

Uncertainty, data assimilation and dynamics in a coastal ecosystem: the Lagoon of Venice. ESSE was used to investigate the seasonal ecosystem dynamics of the Lagoon of Venice in 2001, combining a rich data set with a physical-biogeochemical numerical estuary-coastal model (Cossarini et al, 2008). Novel stochastic modeling components were developed to represent uncertainties in the internal ecosystem dynamics model, measurement model and boundary forcing by rivers, open-sea inlets and industrial discharges. The formulation and parameters of these new additive and multiplicative stochastic error models were optimized based on data-model forecast misfits. The sensitivity to initial and boundary conditions was quantified and analyzed. Half-decay characteristic times were estimated for key ecosystem variables and their spatial and temporal variability studied. The new error models were used in the ESSE scheme for ensemble uncertainty predictions and data assimilation, and an optimal ensemble dimension was estimated. The seasonal biogeochemical-ecosystem fields and their uncertainties were estimated using ESSE and used to guide local environmental policies.

Efficient prognostic equations for ocean uncertainties: New theory and methodologies for representing, evolving and describing large-dimension stochastic ocean flows have been developed. A challenge is to reduce the dimensions of the probability density function fields and to formulate equations for their evolution. Our representation aims to be rich enough to account for essential features but also as efficient as possible to be practical for large-dimension uncertainty computations. Specifically, by constructing a suitable nonlinear transformation we are able to represent efficiently i.e. with low cost and high accuracy, the nonlinear, i.e. non-Gaussian, correlation structure in ocean processes involving uncertainty. This representation combined with existing tools for evolving

uncertainty (ESSE system) allows us to study stochastic, nonlinear interactions between different nonlinear modes of the flow involving different scales and energy spectrum content.

Multi-grid data assimilation into regional tidal models: A new method has been developed for nested data assimilation in barotropic tidal models resolving the topographic and coastal features (Logutov and Lermusiaux, 2008; Logutov, 2008). The method is designed to reduce representativeness errors by fitting the resolved dynamics to data consistently, across a multi-grid computational system. The set of control parameters are presently chosen to be the OBCs of the outer domain. The uncertainty from the outer domain OBCs is propagated to model tidal fields at observation locations through the set of nested domains using efficient low-rank error covariance representations. An analysis increment for these outer OBCs is computed to optimally steer the multi-grid system towards observations by minimizing the (weighted) variance of the observation-minus-forecast residuals.

Scale Estimation Schemes. The knowledge of spatio-temporal scales is fundamental to understand dynamics and is thus useful for a series of applications. In particular, scale estimates are needed in the parameterizations of correlation functions used in steady-state field estimation. Adaptive methods have been implemented to learn the largest and most energetic scales directly from ocean data (prior to mapping these data). The method is based on obtaining the structure function from the available data and utilizing non-linear least square fit to a specified analytical form to estimate the scales in the data. The use of second-generation wavelet analysis is also investigated since it can provide both spatial and temporal scales directly from the data.

Objective Analysis schemes for complex geometries: Our OA scheme which utilizes the Kalman update steps of the Kalman filter has been updated for complex domains. The structure of the correlation function is first specified. Correlation parameters are then obtained using the separation distance estimated from two numerical techniques: a) Level Set Method (LSM) and b) Fast Marching Method (FMM). Knowledge of spatial-time scales provide a measure for the parameters of the analytical correlation function and thus improve field estimates obtained using OA. A third mapping method was also implemented. It uses a numerical diffusion equation to extrapolate the sensor data.

Ocean dynamics, modeling and assimilation: New nesting schemes and open-boundary conditions for nested free-surface primitive-equation ocean models were implemented. New data assimilation schemes for barotropic tidal estimates were published (Logutov and Lermusiaux, 2008). Contributions were made to our Monterey Bay research (Haley et al, 2008; Ramp et al, 2008). A manuscript on the verification and training of models for real-time forecasting was published (Leslie et al, 2008). A special edition of Ocean Dynamics on “Multi-Scale modeling: nested grid and unstructured mesh approaches” was edited with a refereed editorial (Deleersnijder and Lermusiaux, Guest Eds, 2008).

Acoustic predictions. Coupled ocean-acoustic fields were forecast at sea in real-time (Lam et al, 2008). A manuscript on acoustically focused adaptive sampling and onboard routing for marine rapid environmental assessment was completed (Wang et al, 2008). The spatial and temporal variations in acoustic propagation during the PLUSNet07 Exercise in Dabob Bay was described (Xu et al, 2008).

Adaptive sampling. A manuscript on the quantitative planning of the paths of AUVs using Mixed Integer Linear Programming (MILP) was published (Yilmaz et al, 2008). The second part of this work, which selects the ocean sampling paths based on the ESSE-MILP forecasts of data impacts, is finalized (Yilmaz and Lermusiaux, in prep). Schemes for adaptive sampling based on genetic algorithms were evaluated based on Observation System Simulation Experiments (manuscript in prep).

RESULTS

Unstructured Grid Modeling: From the test-cases conducted to evaluate the performance of DGFEM, it was found that low-storage explicit Runge-Kutta schemes with a time discretization limited by the CFL number yields stable, accurate results. Also, using higher order elements on coarser grids resulted in shorter computation times for the same accuracy when compared to finer grids with lower order basis functions. However, coarse-grid, higher-order basis function simulations have fewer degrees of freedom, leading to poorer spatial resolution and the possibility of non-physical features appearing due to Gibbs oscillations. Using variable orders of basis functions for different constituents seems promising as a method to save computational time while retaining accuracy. Preliminary results, shown in Figure 1, indicate that a globally reduced order basis for Zooplankton (in this case) did not significantly affect the result of the simulation.

Efficient prognostic equations for ocean uncertainties: The theoretical framework for the part involving the representation of the probability density function is complete. Specifically, a theoretical proof has been completed in order to show convergence of the proposed method and a numerical algorithm has been tested for simple cases. Progress has also been made on the derivation of reduced order prognostic equations and the development of the corresponding numerical algorithms. Preliminary numerical experiments have also been performed using simple idealized flows, e.g. cavity flow (see Figure 2) and geostrophic turbulence fields (not shown).

Uncertainty, data assimilation and dynamics in a coastal ecosystem: the Lagoon of Venice. The uncertainty analyses show that boundary forcing and internal mixing have a significant control on the seasonal dynamics of the Lagoon of Venice and that data assimilation is needed to reduce their prior uncertainties. Overall, higher uncertainties are predicted in the central and northern regions of the Lagoon. Based on the dominant singular vectors of the ESSE ensemble, the two major northern rivers are the biggest sources of DIN uncertainty in the Lagoon. Other boundary sources such as the southern rivers and industrial discharges can dominate uncertainty modes on certain months. For DIP and phytoplankton, dominant modes are also linked to external boundaries, but internal dynamics effects are more significant than for DIN. Our ESSE estimates of the seasonal biogeochemical fields and their uncertainties in 2001 cover the whole Lagoon (Figure 3) and provide the means to describe the ecosystem and guide local environmental policies (Figure 4). Specifically, our findings and results based on these fields include the: temporal and spatial variability of nutrient and plankton gradients in the Lagoon; dynamical connections among ecosystem fields and their variability; strengths, gradients and mechanisms of the plankton blooms in late-spring, summer and fall; uncertainties of the field predictions, their monthly reductions by data assimilation and thus a quantification of data impacts and data needs; and, finally, an assessment of the water quality in the Lagoon in light of the local environmental legislation.

Multi-grid data assimilation into regional tidal models: Our new methodology based on nested domains in complicated coastal regions allowed fitting the full local tidal data only where it made sense, i.e. where the resolution of the model nests was sufficient to fully resolve the tidal dynamics. The method (Lermusiaux and Logutov, 2008, Logutov, 2008) can avoid artificial steering of the solution towards unresolved observations which is, in general, degrades accuracy. The presence of representativeness errors in data-model misfits was detected through sensitivity experiments with model resolution. In some cases, the observation-minus-forecast residuals were found to be highly sensitive to resolution. For example, in the Phillipines region, a high-resolution (1-minute resolution) nested domain was setup around the Sulu, Bohol, Visayan, and Sibuyan seas, where representativeness

errors were found, and the assimilation of ADCP and Topex/Poseidon data in those areas was carried out using the nested computation. Figure 5 shows the velocities at data location A1 obtained from the 5-min and 1-min resolution runs compared with the depth-averaged ADCP velocity data. The forward solution in the 5-min domain exhibits much larger errors in both amplitude and phase than the forward 1-min resolution nested computations. Figure 6 shows the comparison of the velocity field of the multi-grid inverse solution against the ADCP data. The improvement in the velocity field estimates through the use of our multi-grid inverse can be seen by comparing Figures 6(a) and 5(b).

Scale Estimation Schemes and Objective Analysis schemes for complex geometries: Quantitative scales estimates obtained using our new adaptive learning algorithm are useful. In regions where prior estimates were available, they were found to be in agreement. Our scales estimates are used to guide the scales for objective mapping. With our new OA schemes, coastline constraints are appropriately implemented, i.e. the optimal spatial separation distances are accurately computed such that there is no direct relationship across landforms (islands, peninsulas). The results of the two new OA schemes, the LSM and FMM schemes, were found equivalent, but FMM is less expensive (operation count: $O(N^2 \log N)$) when compared to iteratively obtaining the steady state solution of the Level Set equation with finite difference discretization (operation count: $O(N^3)$). OA maps were compared to maps obtained with the numerical diffusion approach and were found to be in agreement. New schemes to estimate the initial conditions of barotropic transports in complex domains have been implemented.

IMPACT/APPLICATIONS

Better understanding and modeling of physical and interdisciplinary regional ocean dynamics are essential to multiple applications, including efficient real-time at-sea research experiments, naval operations and coastal seas management. Mathematical and computational methods and systems are necessary to predict and study ocean dynamics. Scientific progress occurs from the comparison and optimal combination of measurements and models via data assimilation. Interdisciplinary linkages include the traditional ocean sciences and atmospheric sciences, but also new relationships with other research disciplines within the framework of complex system earth sciences and engineering.

TRANSITIONS

Methods, software and data sets were transitioned to other research groups, several of which were involved in MURI-ASAP, AWACS and PHILEX. They include: MIT-OE, WHOI, Princeton U., NATO Undersea Research Centre (NURC), NRL-Stennis, NPS, OASIS Inc., OGS-Trieste (Italy), CNR-Ancona (Italy), Cal. Tech, U. of Frankfurt (Germany), Rutgers and Duke U.

RELATED PROJECTS

Without the present effort, several other projects would not be feasible. In particular, this project contributed to MURI-ASAP (MIT-sub-00000917), AWACS (N00014-07-1-0501) and PHILEX (N00014-07-1-0473). Interactions also occurred with other research groups. For data assimilation, adaptive sampling and adaptive modeling, this involved: MIT-OE/EAPS (N. Patrikalakis, H. Schmidt, C. Evangelinos), OASIS Inc. (K. Heaney), NURC (M. Rixen), NRL-Stennis (E. Coelho) and U. Mass (A. Gangopadhyay). For physical-biogeochemical studies, collaborations involved J. McCarthy (HU) and for Mediterranean studies, NURC, U. Ancono (N. Russo), F-P. Lam (TNO) and U. Trieste (G. Cosarini, C. Solidoro).

PUBLICATIONS (2008)

Cossarini, G., P.F.J. Lermusiaux and C. Solidoro, 2008. Uncertainty Analyses, Error Subspace Data Assimilation and Seasonal Dynamics in a Coastal Ecosystem: the Lagoon of Venice. *Journal of Geophysical Research* [submitted, refereed].

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Xu, J., P.F.J. Lermusiaux, P.J. Haley Jr., W.G. Leslie and O.G. Logutov, 2008. Spatial and temporal variations in acoustic propagation during the PLUSNet07 exercise in Dabob Bay. *Proc. of Meetings on Acoustics (POMA)*, Vol. 4, 155th Meeting Acoustical Society of America [published, refereed]

Yilmaz, N.K., C. Evangelinos, P.F.J. Lermusiaux and N. Patrikalakis, 2008. Path Planning of Autonomous Underwater Vehicles for Adaptive Sampling Using Mixed Integer Linear Programming. *IEEE Ocean Engineering* [in press, refereed].

Additional presentations and other publications are available from <http://mseas.mit.edu/>. Other specific figures are available upon request.

FIGURES

Figure 1: Idealized biogeochemical simulations with variable orders basis functions

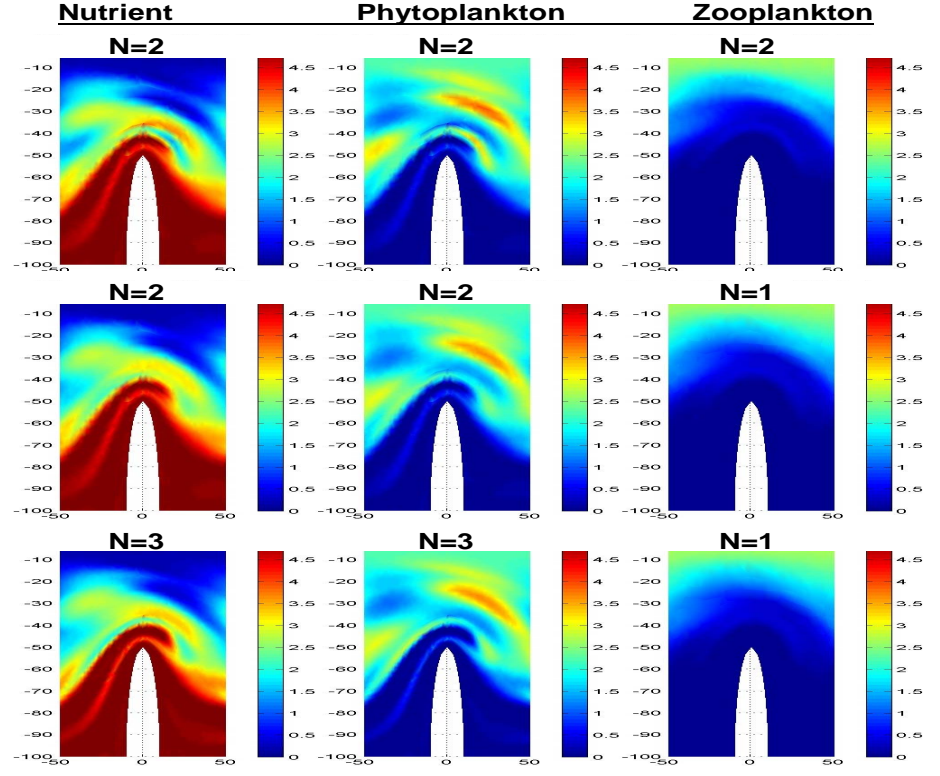
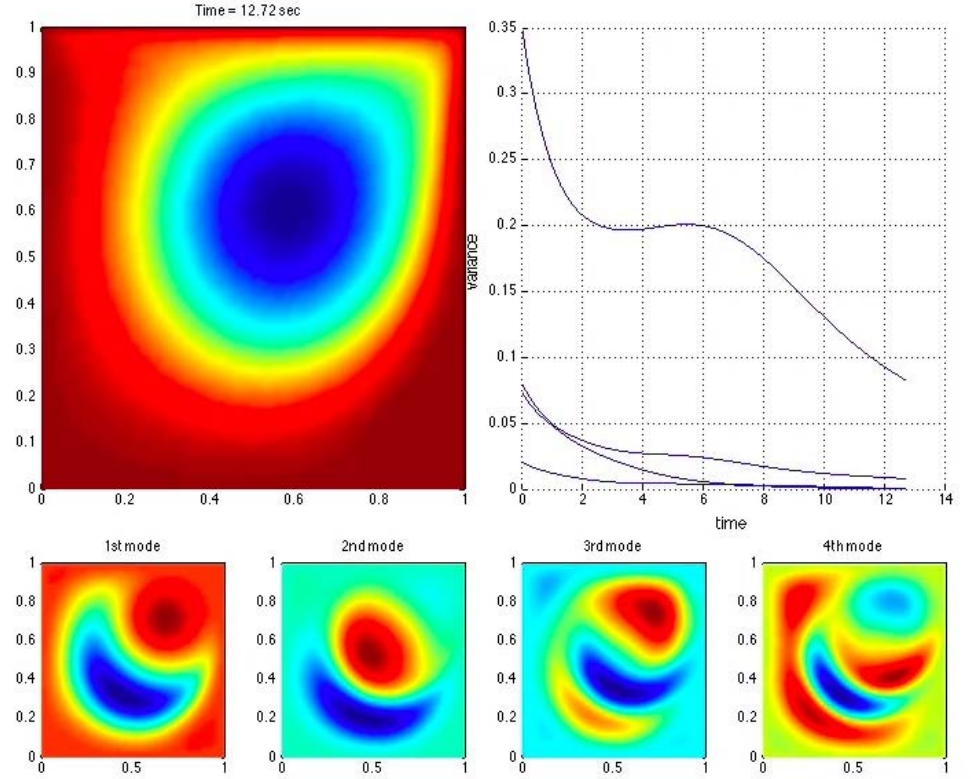


Figure 2: Cavity flow with random initial conditions. Upper left plot: Mean stream-function. Upper right: Variance evolution of each of the nonlinear modes. Lower plots: Instantaneous plots of the stream-functions describing the first four more energetic stochastic modes.



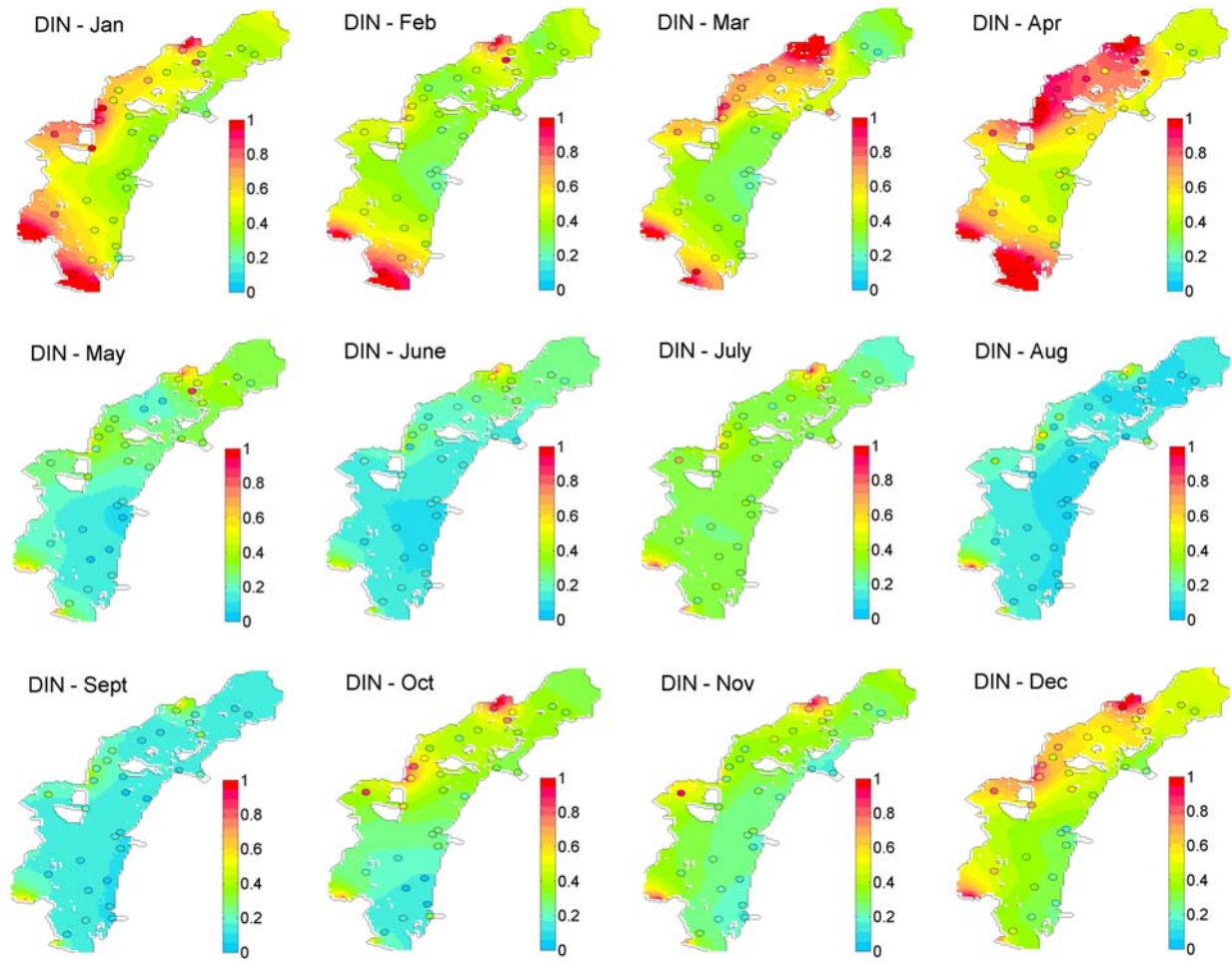


Figure 3. Evolution of the *a posteriori* fields for DIN [mg/l] (maps), and observation (overlaid colored circles) for the Lagoon of Venice in 2001. Color scale is set to 0 to 1 mg/l for all months.

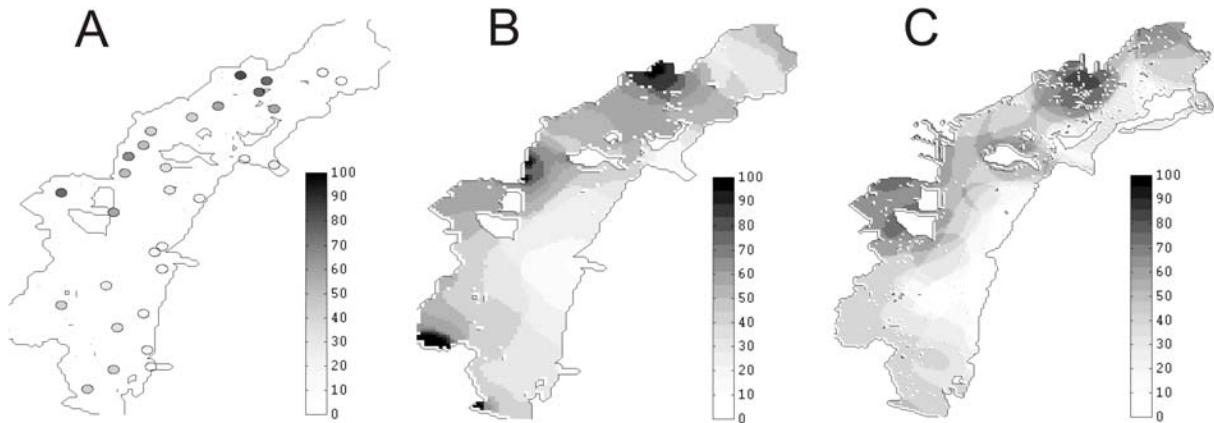
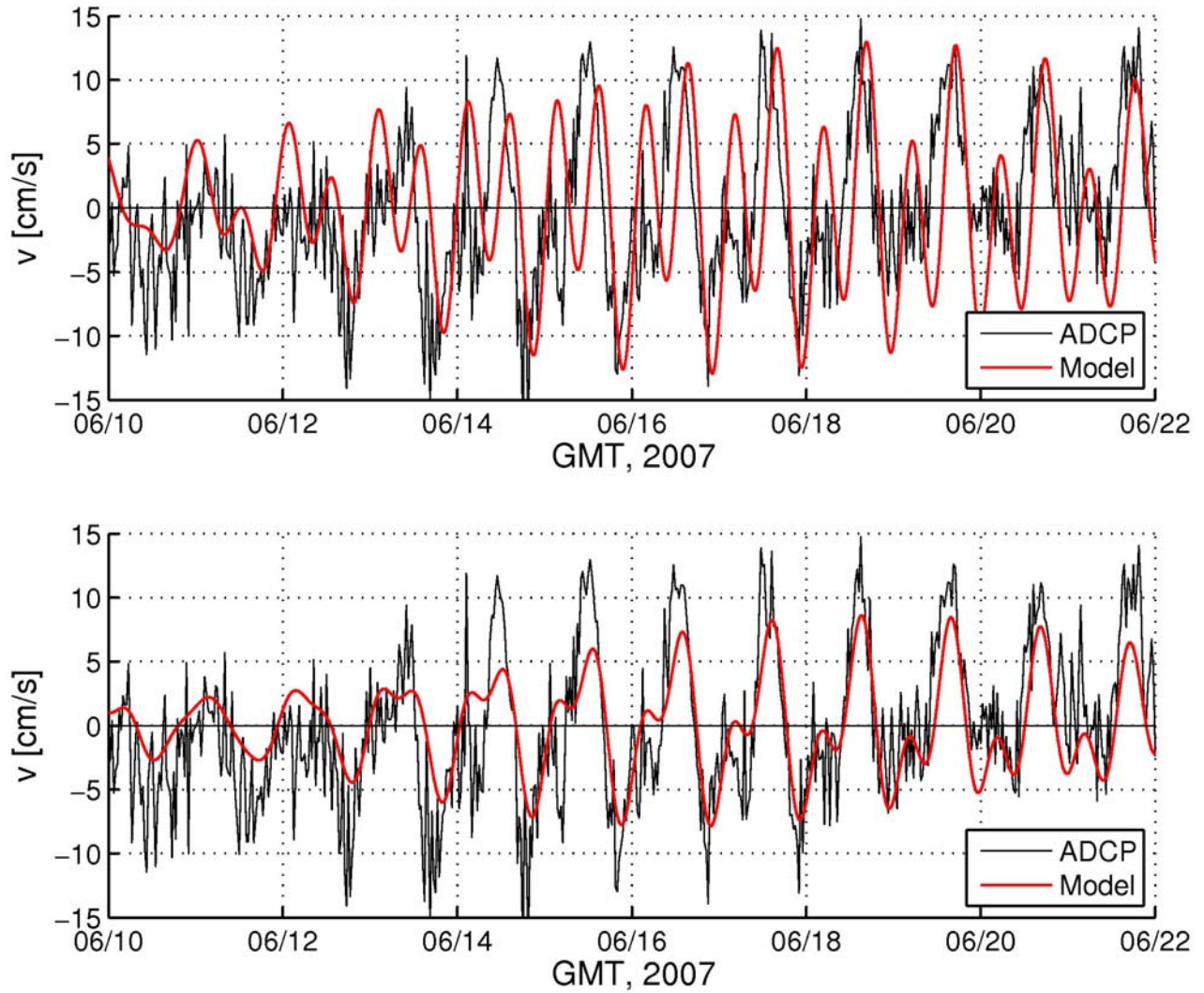


Figure 4. Percentage of time of the year during which the Lagoon of Venice is above the limit of the Water Quality Target for DIN. (a) data, (b) OA estimate, (c) ESSE estimate.

Figure 5: Observed and forward model velocity at data location A1 (see Logutov, 2008). Observed



meridional depth-averaged velocity, with mean removed (black). Model velocity (red). (Top) at 5-min resolution; (Bottom) at 1-min resolution.

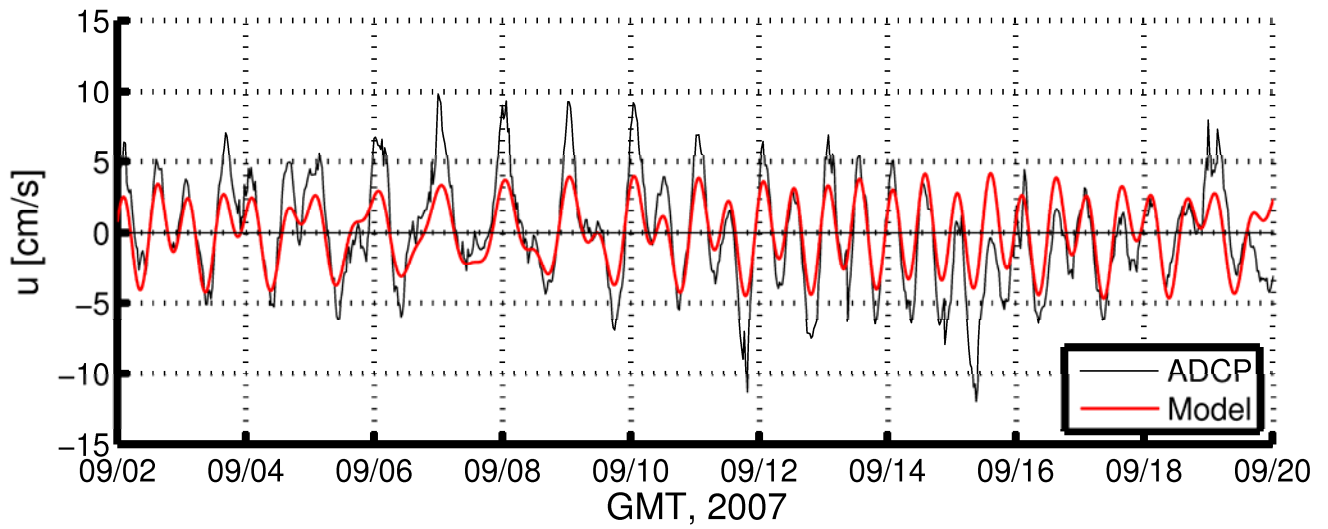
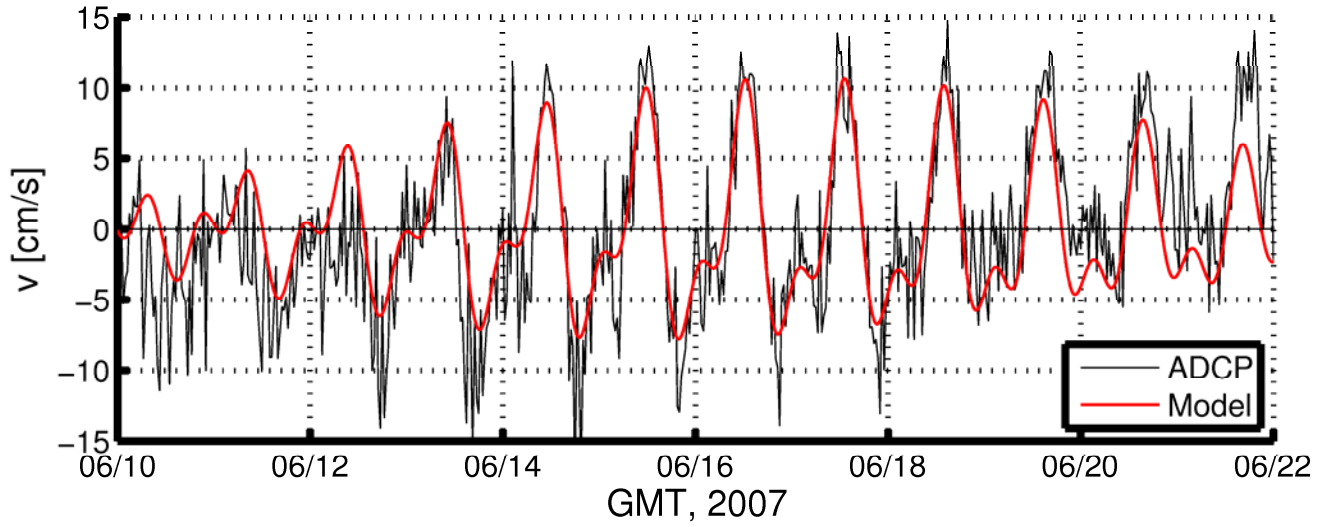


Figure 6: Observed versus inverse model velocities at A1 and A2. Plotted are the depth-averaged velocities, with mean removed. (Top) meridional velocity at A1; (Bottom) zonal velocity at A2.